19. (Four Times Amended) A method of using a computer for evaluating the ability of at least one of a plurality of chemical entities to associate with a crystallized molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;
wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a) positioning a graphical three-dimensional representation of the structure of one of said plurality of chemical entities within the CnA binding pocket or the CnA homologue binding pocket;

b) performing a fitting operation between said graphical representation of the structure of said chemical entity and the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said graphical representation of the structure and said structure coordinates;

c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

d) outputting said quantified association to a suitable output hardware;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

20. (Four Times Amended) A method of using a computer for evaluating the ability of at least one of a plurality of chemical entities to associate with a crystallized

molecule or molecular complex comprising a CnA binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a) positioning a graphical three-dimensional representation of the structure of one of said plurality of chemical entities within the CnA binding pocket or the CnA homologue binding pocket;

b) performing a fitting operation between said graphical representation of the structure of said chemical entity and the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said graphical representation of the structure and said structure coordinates;

c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

d) outputting said quantified association to a suitable output hardware;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

21. (Four Times Amended) A method of using a computer for evaluating the ability of at least one of a plurality of chemical entities to associate with a crystallized molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344,

345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a) positioning a graphical three-dimensional representation of the structure of one of said plurality of chemical entities within the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b) performing a fitting operation between said graphical representation of the structure of said chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said graphical representation of the structure and said structure coordinates;

c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

d) outputting said quantified association to a suitable output hardware;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.